4-Trifluoromethylpiperidine

Inchi: InChI=1S/C6H10F3N/c7-6(8,9)5-1-3-10-4-2-5/h5,10H,1-4H2
InchiKey: RDRQUUWCJTYHCT-UHFFFAOYSA-N
Formula: C6H10F3N
SMILES: FC(F)(F)C1CCNCC1
Mol. weight [g/mol]: 153.15
CAS: 657-36-3

Physical Properties

Property code	Value	Unit	Source
affp	925.10	kJ/mol	NIST Webbook
basg	892.00	kJ/mol	NIST Webbook
gf	-469.79	kJ/mol	Joback Method
hf	-672.12	kJ/mol	Joback Method
hfus	14.55	kJ/mol	Joback Method
hvap	32.39	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.548		Crippen Method
mcvol	99.830	ml/mol	McGowan Method
pc	3543.08	kPa	Joback Method
tb	399.36	K	Joback Method
tc	592.13	K	Joback Method
tf	273.98	K	Joback Method
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.73	J/mol×K	399.36	Joback Method
cpg	215.40	J/mol×K	431.49	Joback Method
cpg	229.29	J/mol×K	463.62	Joback Method
cpg	242.42	J/mol×K	495.74	Joback Method
cpg	254.80	J/mol×K	527.87	Joback Method
cpg	266.48	J/mol×K	560.00	Joback Method
cpg	277.47	J/mol×K	592.13	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C657363&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume